Determination of Temperature Profile of Processes for Oxidative Dehydrogenation of Hydrocarbons

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Creating an effective apparatus for universal feedstock is one of the most important problems in the materials development processes, particularly in the petrochemical and chemical industries. In this paper, we present the results of a study of the problem of optimal hardware design for hydrocarbon processing. As an example, we examined the process of oxidative dehydrogenation (ODH) of n-butane to butadiene. Theoretically optimal temperature profile (TOTP) was defined. We applied Pontryagin's maximum principle, which takes into account the maximum output of desired product. Mathematical model of the kinetics of ODH of n-C4H10 to butadiene was considered. The results show that changes in the initial partial pressure of n-C4H10 in (3-6 kPa) range increase the output of butadiene from 22.4% to 26%. Further increase in the initial partial pressure of n-C4H10 from 6 to 9 kPa decreases the output of the desired product to 23%. At the initial partial pressure of n-C4H10 3 kPa, increase in the initial partial pressure of oxygen (PO2) leads to decrease in the output of butadiene from 25.3% at PO2 = 2 kPa to 22% at PO2 = 7 kPa; and to 16% at PO2 = 12 kPa. Numerical solution of TOTP problem has revealed the existence of optimal region of regime parameters for ODH of hydrocarbons. We found the principal possibility of conducting the process of ODH of n-C4H10 to butadiene in an adiabatic reactor with intermediate heat removal and section-by-section feed.